

Recent progresses on diagrammatic determinant QMC

Lei Wang, ETH Zürich

Trento 2015.io



better scaling

Iazzi and Troyer, PRB 2015

LW, Iazzi, Corboz and Troyer, PRB 2015



entanglement & fidelity

LW and Troyer, PRL 2014

LW, Liu, Imriška, Ma and Troyer, PRX 2015

LW, Shinaoka and Troyer, PRL 2015



sign problem

Huffman and Chandrasekharan, PRB 2014

Li, Jiang and Yao, PRB 2015

LW, Liu, Iazzi, Troyer and Harcos, PRL 2015

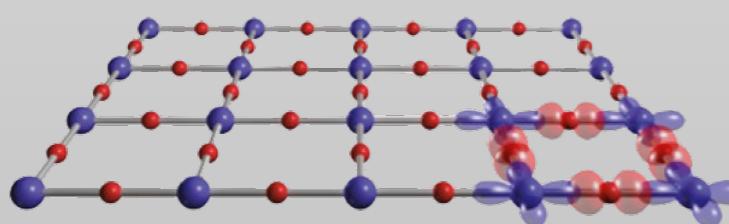
About me

- Background: condensed matter physics

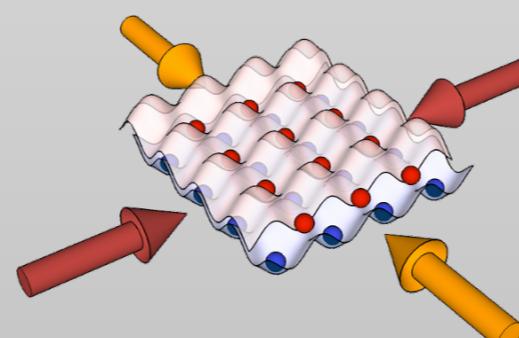
Please forgive my ignorance!

- Interested in quantum many-body systems, quantum phase transitions, etc

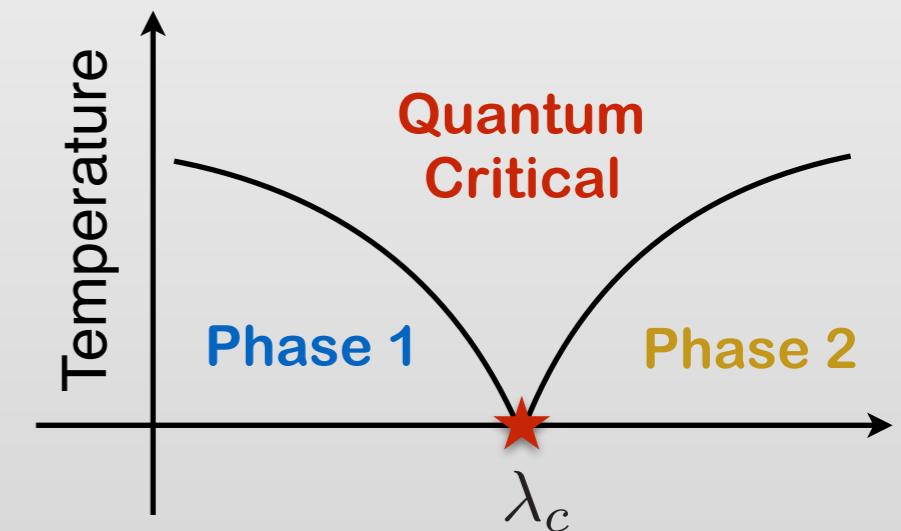
- Hubbard model of fermions in this talk



Solid materials

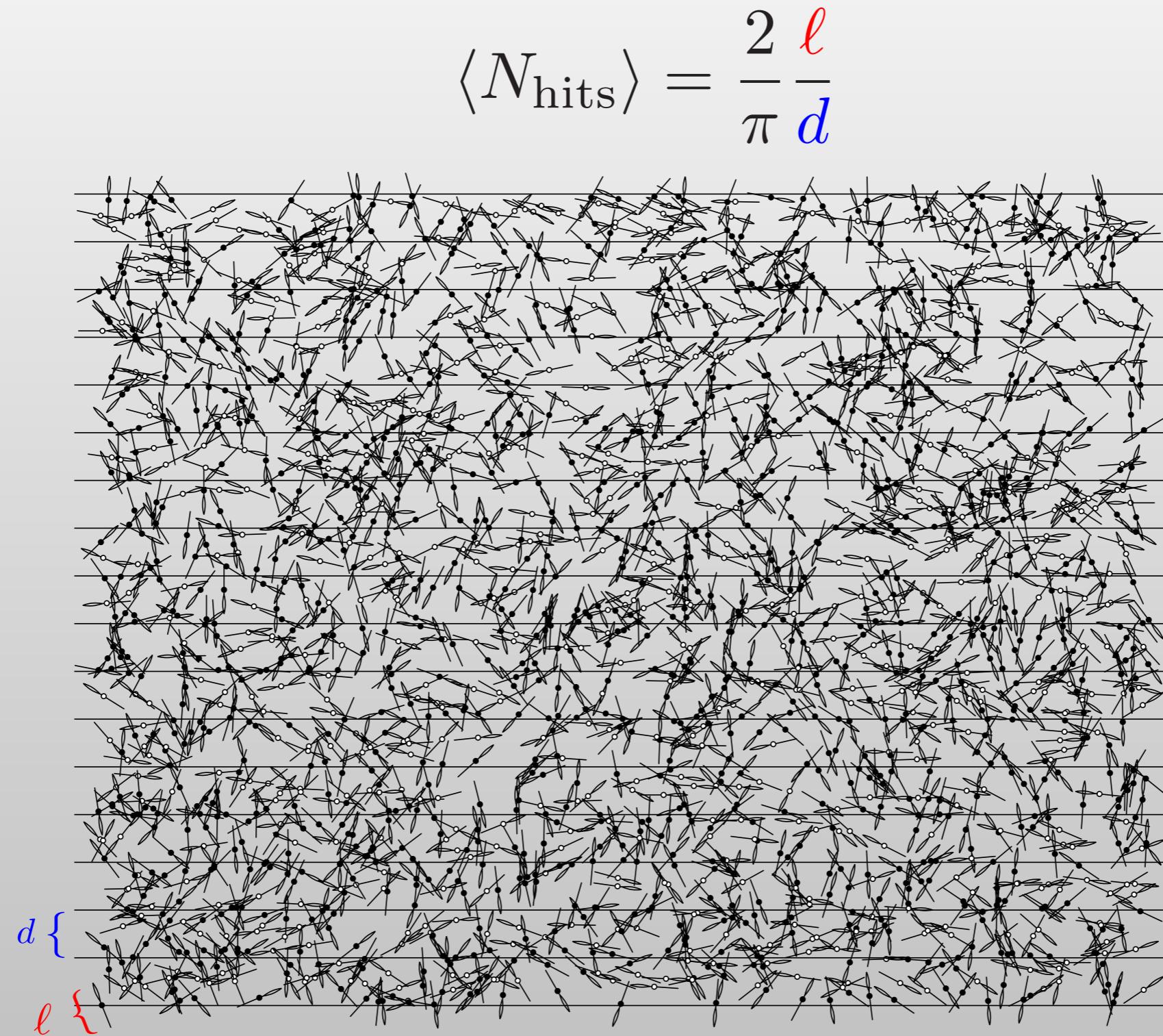


Optical lattices



Quantum Monte Carlo

The first recorded Monte Carlo simulation



Buffon 1777

Statistical Mechanics:
Algorithms and Computations
Werner Krauth

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

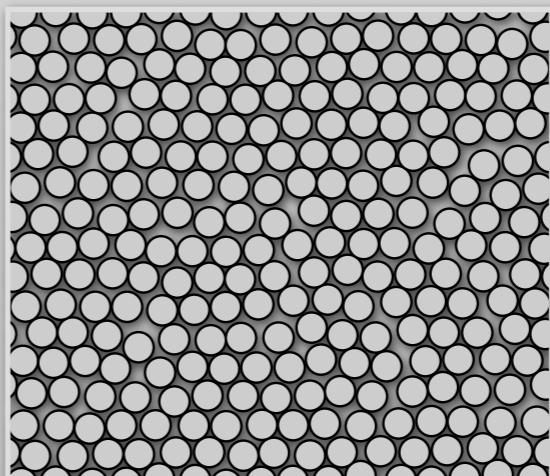
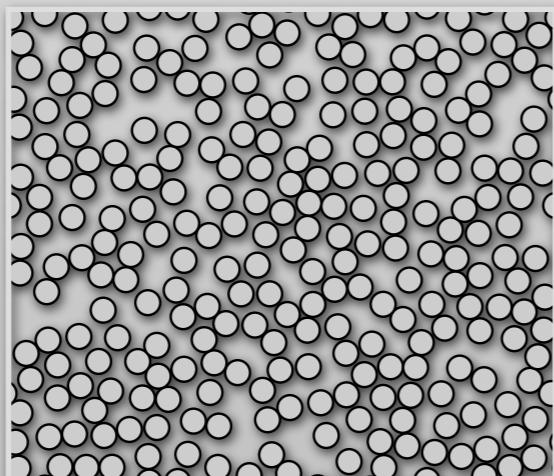
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed,

II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† containing N particles.

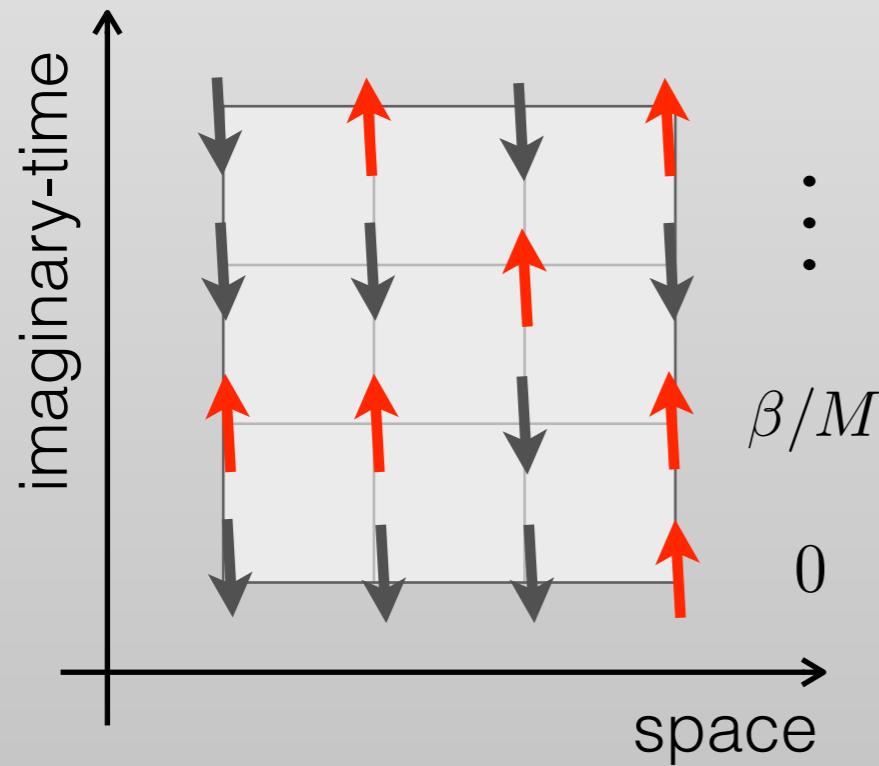


Quantum to classical mapping

$$Z = \text{Tr} \left(e^{-\beta \hat{H}} \right) \quad \hat{H} = \hat{H}_0 + \lambda \hat{H}_1$$

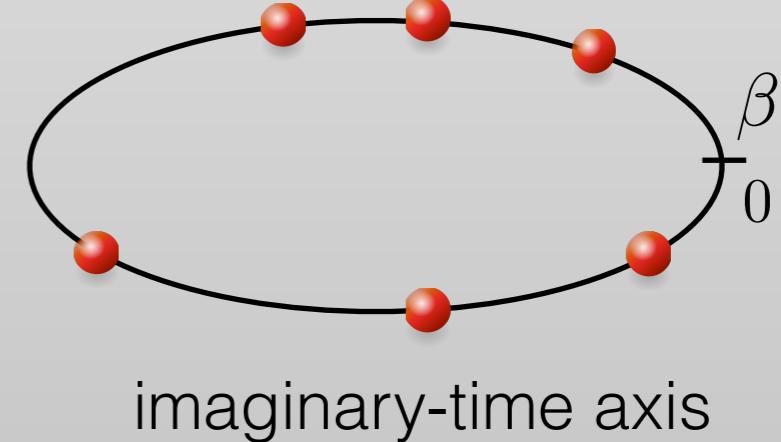
Trotterization

$$Z = \text{Tr} \left(e^{-\frac{\beta}{M} \hat{H}} \dots e^{-\frac{\beta}{M} \hat{H}} \right)$$



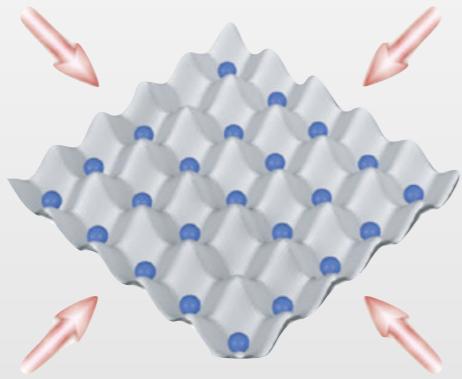
Diagrammatic approach

$$Z = \sum_{k=0}^{\infty} \lambda^k \int_0^{\beta} d\tau_1 \dots \int_{\tau_{k-1}}^{\beta} d\tau_k \times \text{Tr} \left[(-1)^k e^{-(\beta-\tau_k) \hat{H}_0} \hat{H}_1 \dots \hat{H}_1 e^{-\tau_1 \hat{H}_0} \right]$$



Beard and Wiese, 1996
Prokof'ev, Svistunov, Tupitsyn, 1996

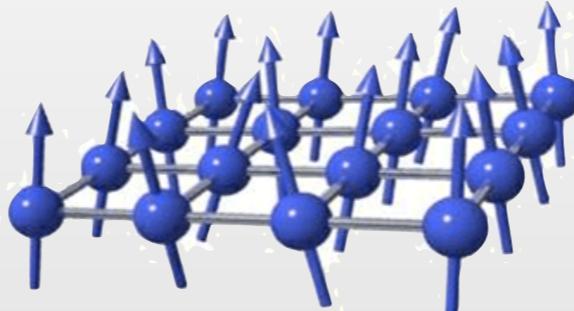
Diagrammatic approaches



bosons

World-line Approach

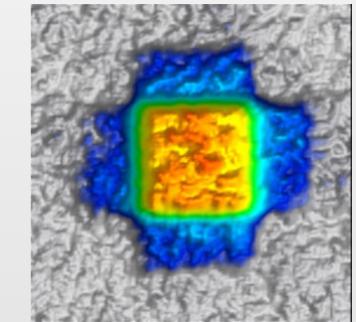
Prokof'ev et al, JETP, **87**, 310 (1998)



quantum spins

Stochastic Series Expansion

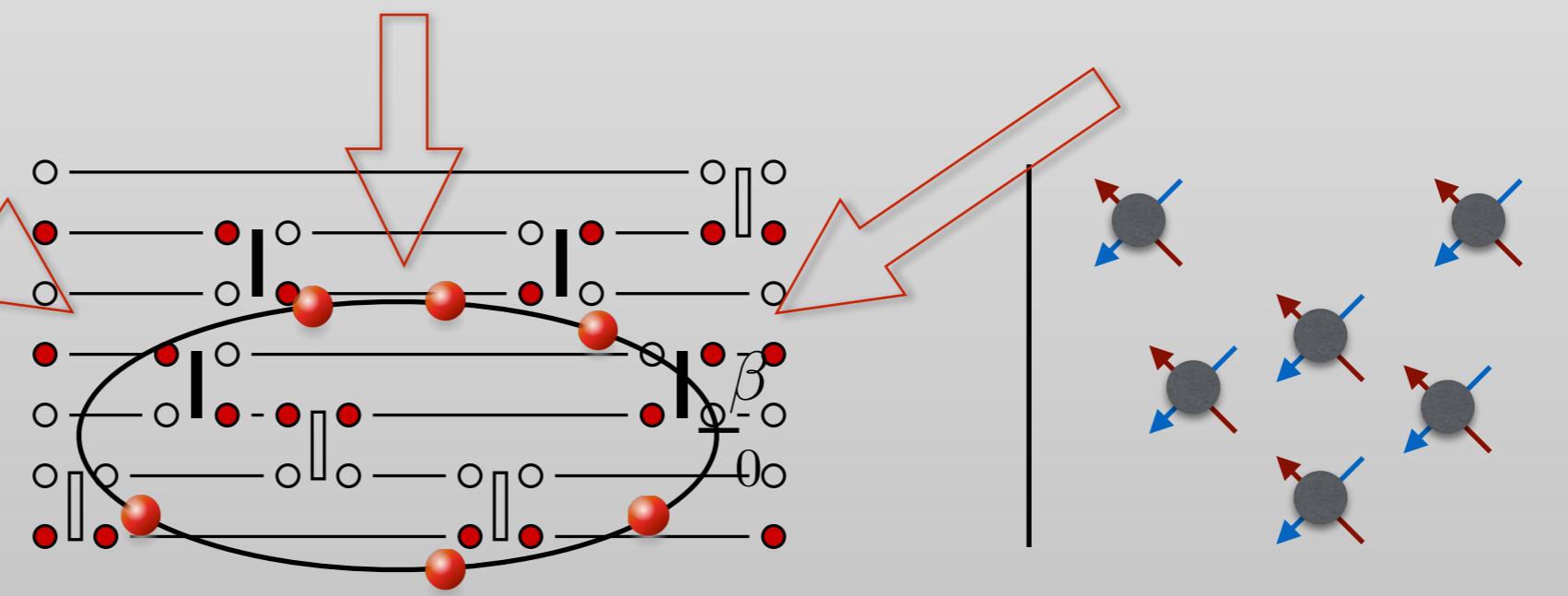
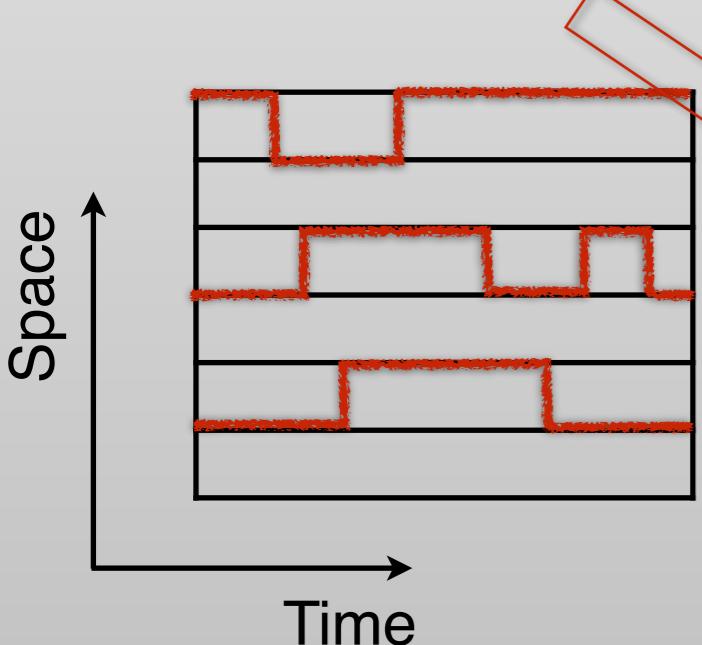
Sandvik et al, PRB, **43**, 5950 (1991)



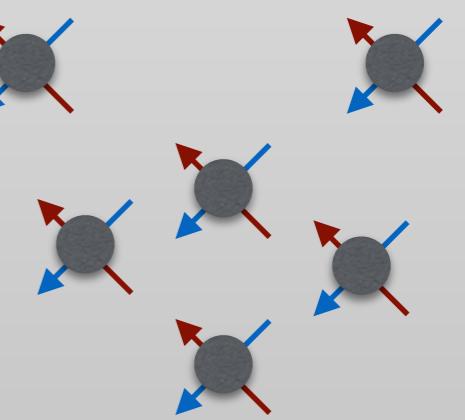
fermions

Determinantal Methods

Gull et al, RMP, **83**, 349 (2011)



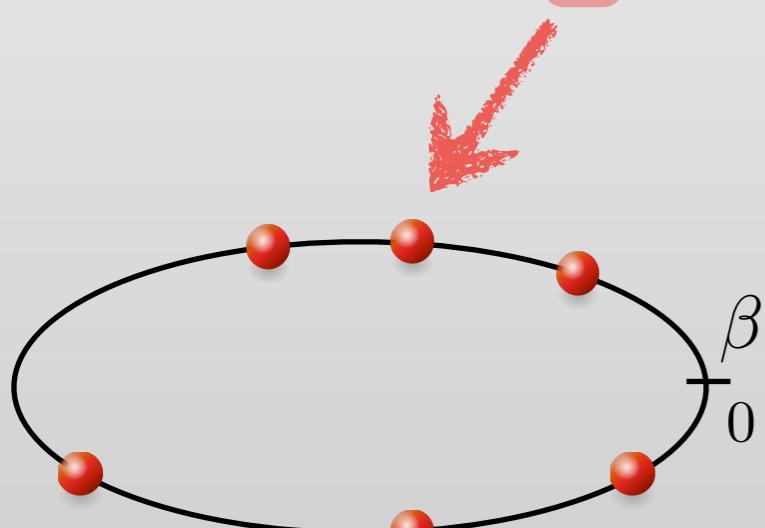
|



Diagrammatic determinant QMC

$$Z = \sum_{k=0}^{\infty} \lambda^k \int_0^{\beta} d\tau_1 \dots \int_{\tau_{k-1}}^{\beta} d\tau_k \text{Tr} \left[(-1)^k e^{-(\beta-\tau_k)\hat{H}_0} \hat{H}_1 \dots \hat{H}_1 e^{-\tau_1 \hat{H}_0} \right]$$

$$= \sum_{k=0}^{\infty} \lambda^k \sum_{\mathcal{C}_k} w(\mathcal{C}_k)$$



Rubtsov et al, PRB 2005 Gull et al, RMP 2011

$$\det \left(\begin{array}{c} \text{Noninteracting} \\ \text{Green's functions} \end{array} \right)_{k \times k}$$

$$\langle k \rangle \sim \beta \lambda N, \text{ scales as } \mathcal{O}(\beta^3 \lambda^3 N^3)$$

Rombouts, Heyde and Jachowicz, PRL 1999
Iazzi and Troyer, PRB 2015 LW, Iazzi, Corboz and Troyer, PRB 2015

**LCT-QMC
Methods**



$$\det \left(I + \mathcal{T} e^{-\int_0^{\beta} d\tau H_{\mathcal{C}_k}(\tau)} \right)_{N \times N}$$

thus achieving $\mathcal{O}(\beta \lambda N^3)$ scaling!

Fidelity susceptibility made simple!

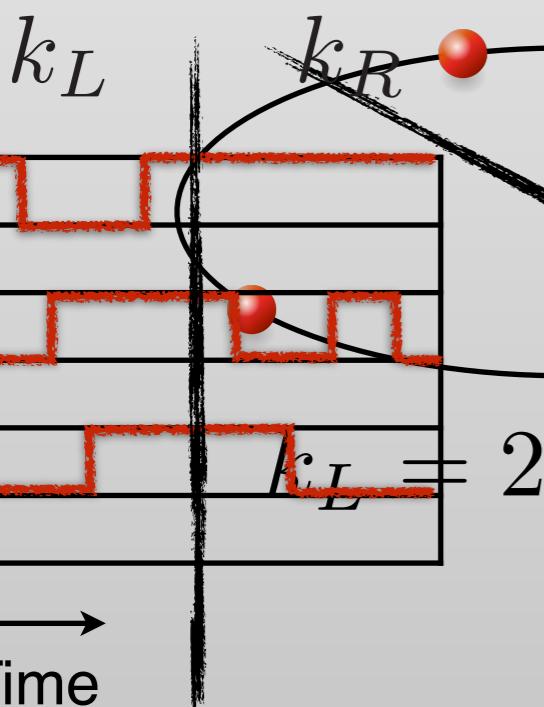
LW, Liu, Imriška, Ma and Troyer, PRX 2015

$$\chi_F = \frac{\langle k_L k_R \rangle - \langle k_L \rangle \langle k_R \rangle}{2\lambda^2}$$

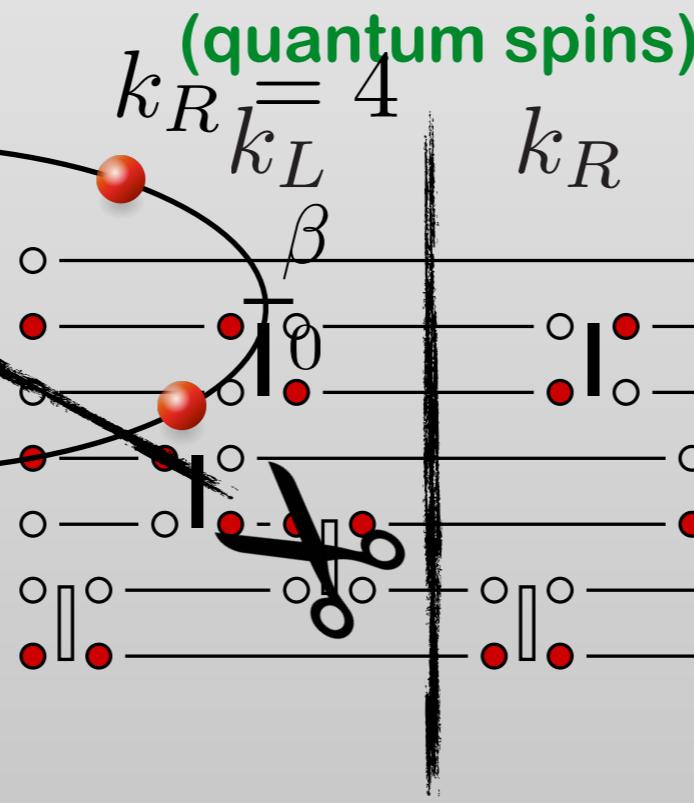
Signifies quantum phase transitions without need of the local order parameter

Worldline Algorithms Stochastic Series Expansion Determinantal Methods

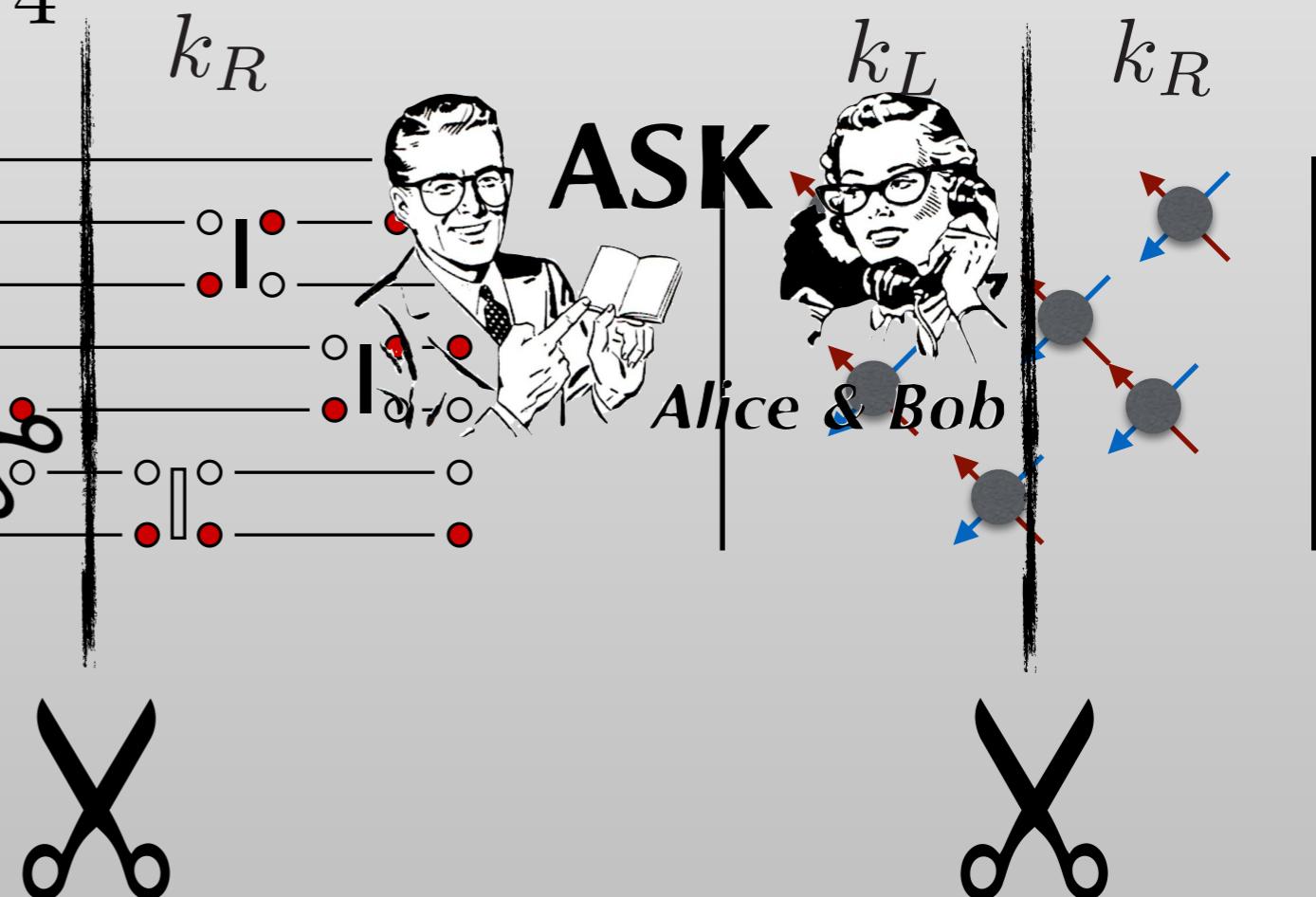
(bosons)



(quantum spins)



(fermions)



More advantages

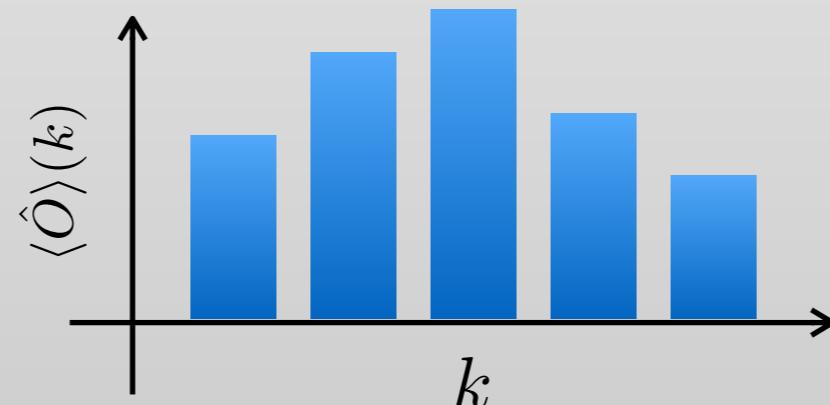
$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_k \lambda^k \sum_{\mathcal{C}_k} w(\mathcal{C}_k) O(\mathcal{C}_k)$$

Observable derivatives

$$\frac{\partial \langle \hat{O} \rangle}{\partial \lambda} = \frac{\langle \hat{O} k \rangle - \langle \hat{O} \rangle \langle k \rangle}{\lambda}$$

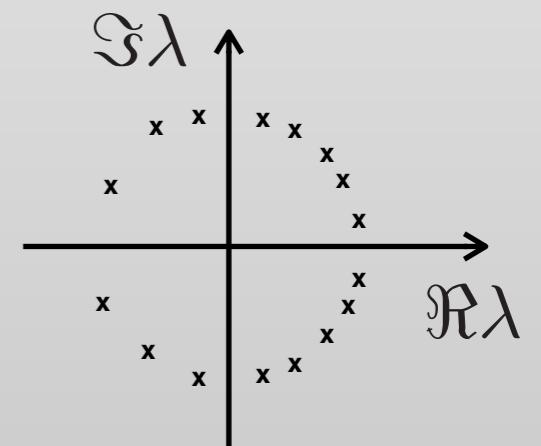
Directly sample *derivatives* of any observable

Histogram reweighing



Can obtain observables in a *continuous range* of coupling strengths

Lee-Yang zeros



Partition function zeros in the *complex coupling strength* plane

What about the sign problem ?



Sign problem free: Kramers pairs due to the time-reversal symmetry

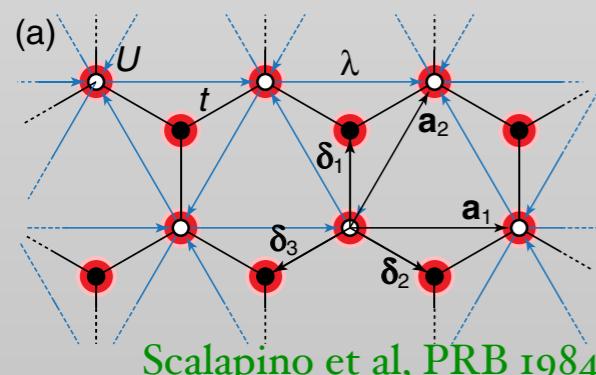
$$M_{\uparrow} = M_{\downarrow}^*$$

$$\begin{aligned} w(\mathcal{C}_k) &= \det M_{\uparrow} \times \det M_{\downarrow} \\ &= |\det M_{\uparrow}|^2 \geq 0 \end{aligned}$$

Lang et al, Phys. Rev. C, 1993
 Koonin et al, Phys. Rep., 1997
 Hands et al, EPJC, 2000
 Wu et al, PRB, 2005

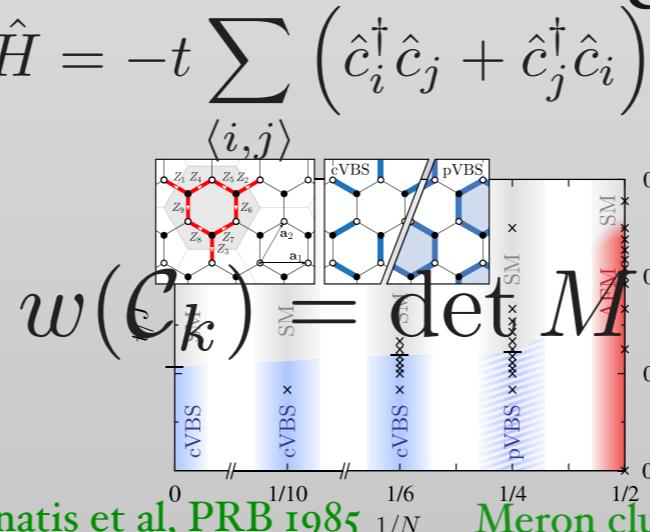


Attractive interaction at any filling on any lattice
 But, how about this?
 Repulsive interaction at half-filling on bipartite lattices
 spinless fermions
 And more ...

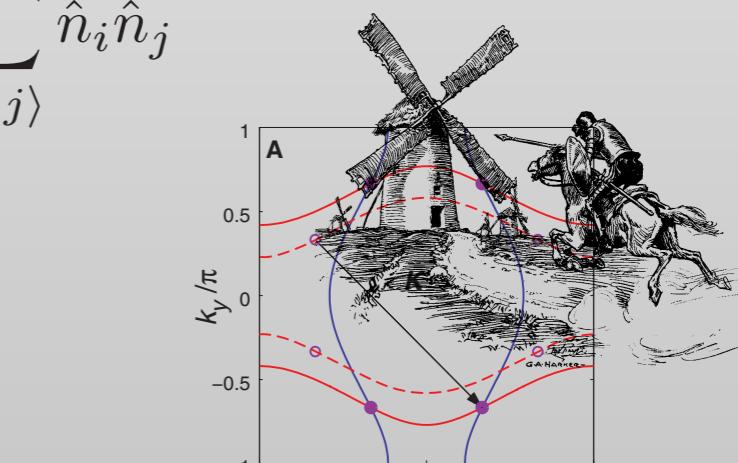


Topological insulators and $SU(2N)$ models

Hohenadler, Lang and Assaad, PRL 2011



Gubernatis et al, PRB 1985 Meron cluster approach, Chandrasekharan and Wiese, PRL 1999



Berg, Metliski and Sachdev, Science 2012

Lang, Meng, Muramatsu, Wessel and Assaad, PRL 2013

Solutions !

PHYSICAL REVIEW B **89**, 111101(R) (2014)

Solution to sign problems in half-filled spin-polarized electronic systems

Emilie Fulton Huffman and Shailesh Chandrasekharan

Department of Physics, Duke University, Durham, North Carolina 27708, USA

(Received 19 December 2013; revised manuscript received 14 February 2014; published 12 March 2014)



PHYSICAL REVIEW B **91**, 241117(R) (2015)



Solving the fermion sign problem in quantum Monte Carlo simulations by Majorana representation

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³*Collaborative Innovation Center of Quantum Matter, Beijing 100084, China*

(Received 27 August 2014; revised manuscript received 13 October 2014; published 30 June 2015)

PHYSICAL REVIEW B **91**, 235151 (2015)



Efficient continuous-time quantum Monte Carlo method for the ground state of correlated fermions

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¹*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*

²*Institute for Theoretical Physics, University of Amsterdam, Science Park 904 Postbus 94485, 1090 GL Amsterdam, The Netherlands*

(Received 12 January 2015; revised manuscript received 13 March 2015; published 30 June 2015)

1506.05349

Split orthogonal group:

A guiding principle for sign-problem-free fermionic simulations

Lei Wang¹, Ye-Hua Liu¹, Mauro Iazzi¹, Matthias Troyer¹ and Gergely Harcos²

¹*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland and*

²*Alfréd Rényi Institute of Mathematics, Reáltanoda utca 13-15., Budapest H-1053, Hungary*

A tale of open science

News & Comment

News

2015

September

Article

NATURE | BREAKING NEWS



Maths whizz solves a master's riddle

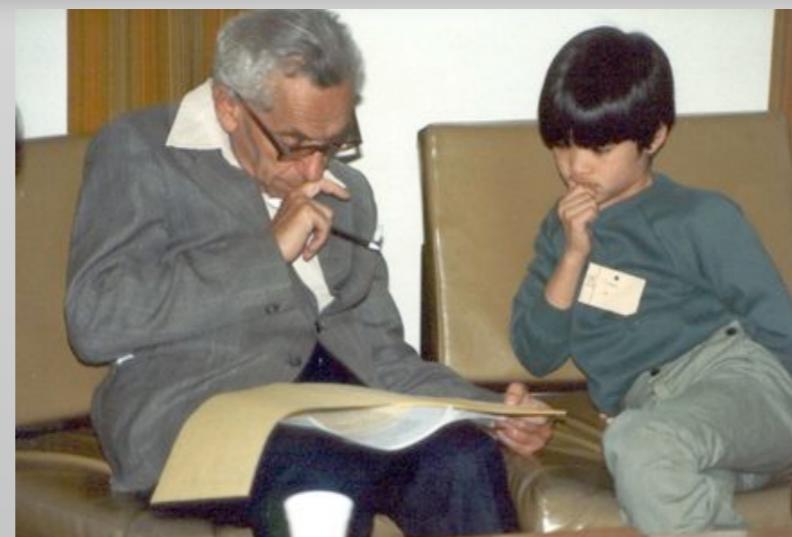
Terence Tao successfully attacks the Erdős discrepancy problem by building on an online collaboration.

Chris Cesare

25 September 2015

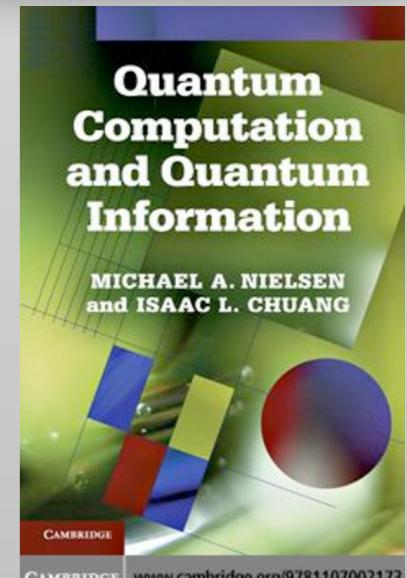
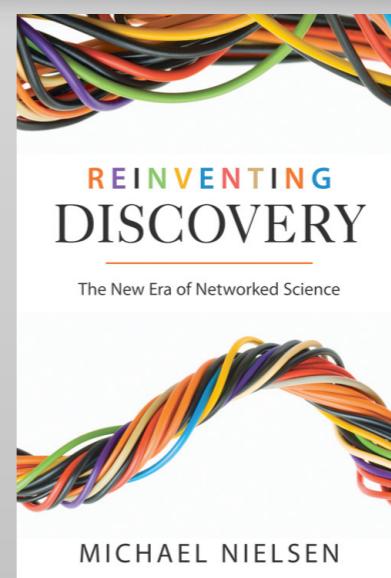
math**overflow**

The conjecture was proved by Gergely Harcos and Terence Tao, with inputs from others



Tao and Paul Erdős in 1985

<https://terrytao.wordpress.com/2015/05/03/the-standard-branch-of-the-matrix-logarithm/>



A new de-sign principle

LW, Liu, Iazzi, Troyer and Harcos 1506.05349

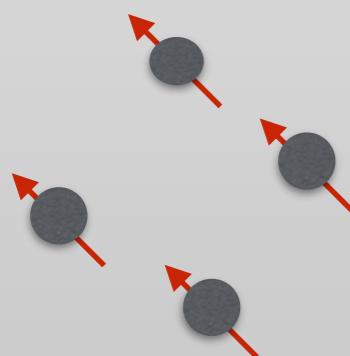
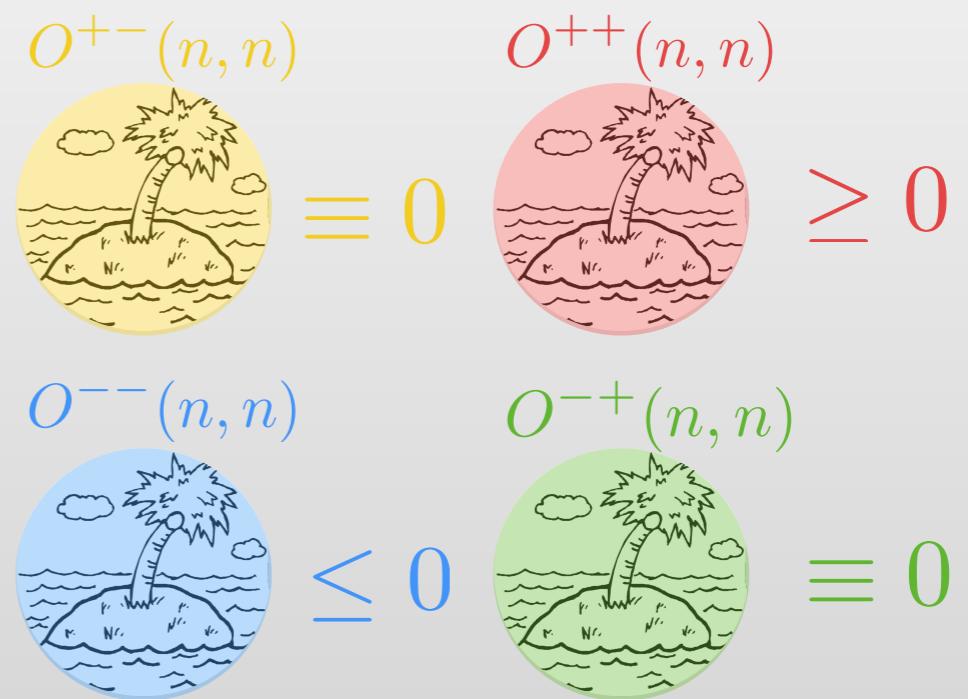
If $M^T \eta M = \eta$ where $\eta = \text{diag}(I, -I)$

Then

$$\det \in IO(M, \eta)$$

$\mathcal{T} e^{-\int_0^\beta d\tau H c_k(\tau)}$

has a orthogonal group
for each component !



spinless fermions

LW, Troyer, PRL 2014

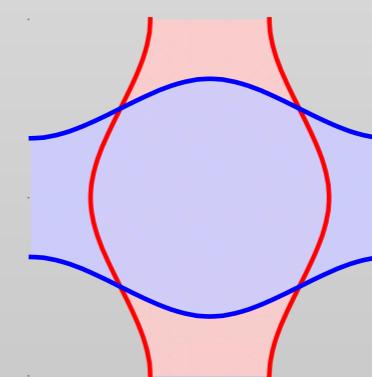
LW, Corboz, Troyer, NJP 2014

LW, Iazzi, Corboz, Troyer, PRB, 2015

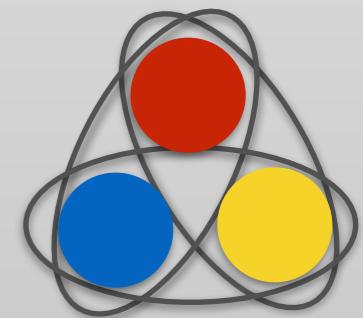


split Dirac cone

Liu and LW, 1510.00715

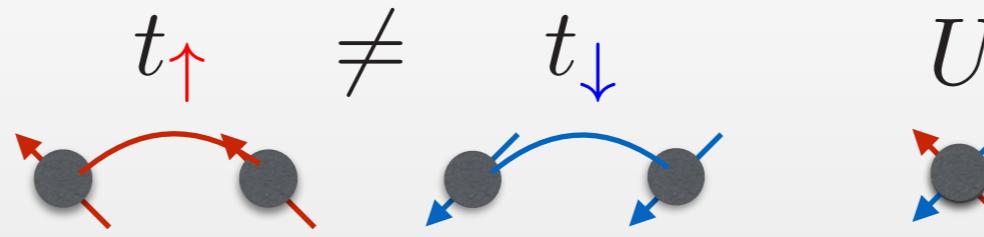


spin nematicity



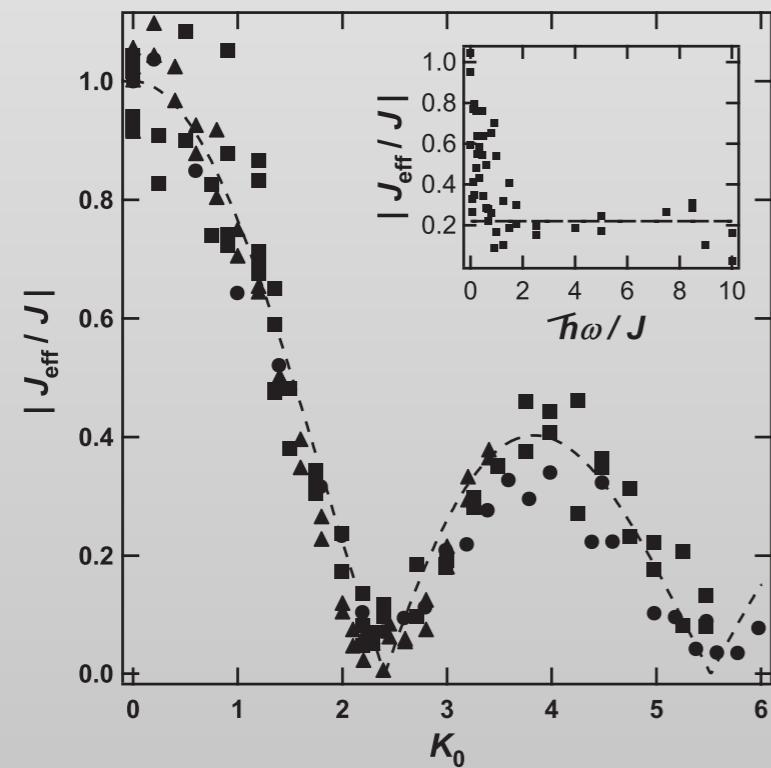
SU(3)

Asymmetric Hubbard model

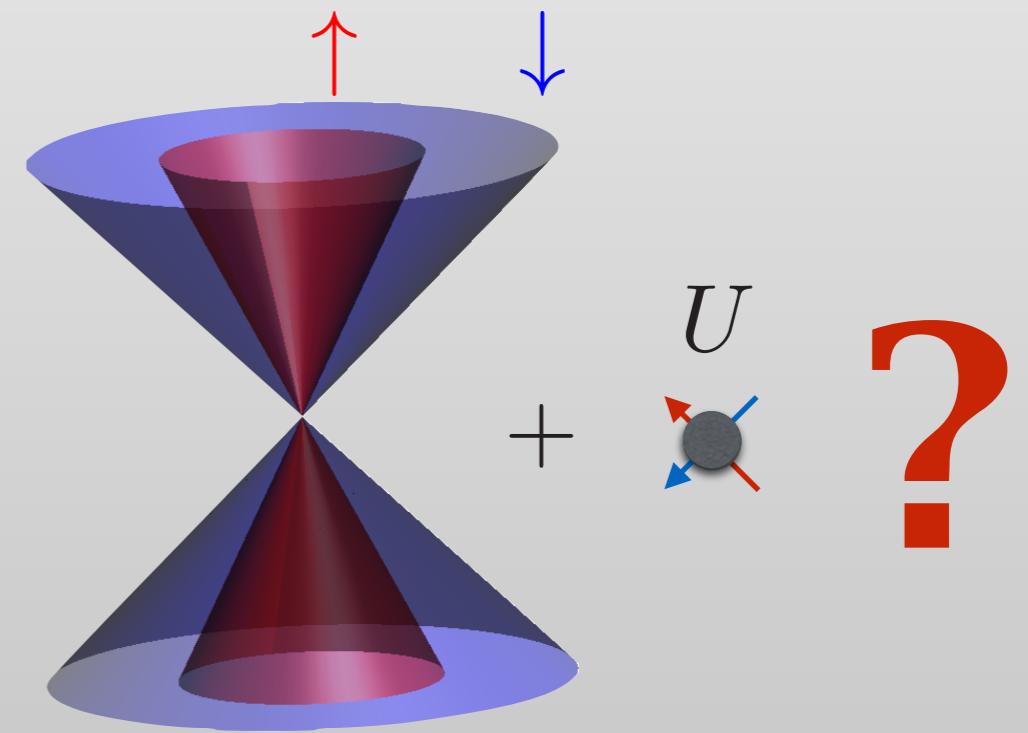


- Realization: mixture of ultracold fermions (e.g. ${}^6\text{Li}$ and ${}^{40}\text{K}$)
- Now, continuously tunable by **spin-dependent modulations** Jotzu et al, PRL 2015

$$t_{\downarrow}/t_{\uparrow} \in (-\infty, \infty)$$

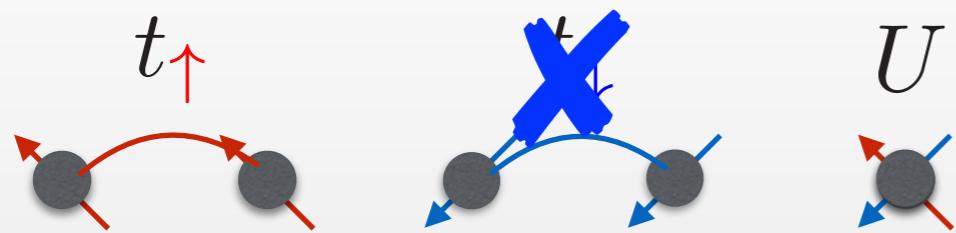


Lignier et al, PRL 2007 and many others

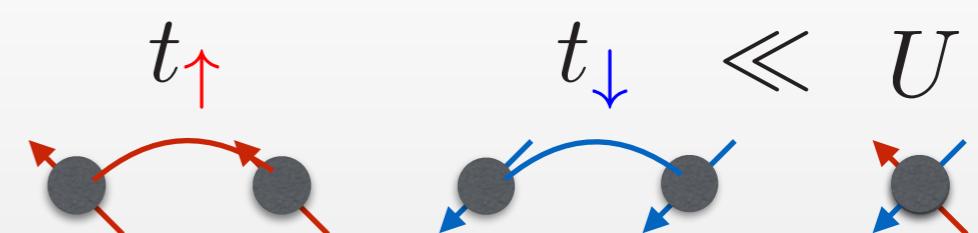


Dirac fermions with unequal Fermi velocities

Two limiting cases



Falicov-Kamball Limit



Strong Coupling Limit

SIMPLE MODEL FOR SEMICONDUCTOR-METAL TRANSITIONS:
 SmB_6 AND TRANSITION-METAL OXIDES

L. M. Falicov*

Department of Physics, University of California, Berkeley, California 94720

and

J. C. Kimball†

Department of Physics, and The James Franck Institute, University of Chicago, Chicago, Illinois 60637
(Received 12 March 1969)

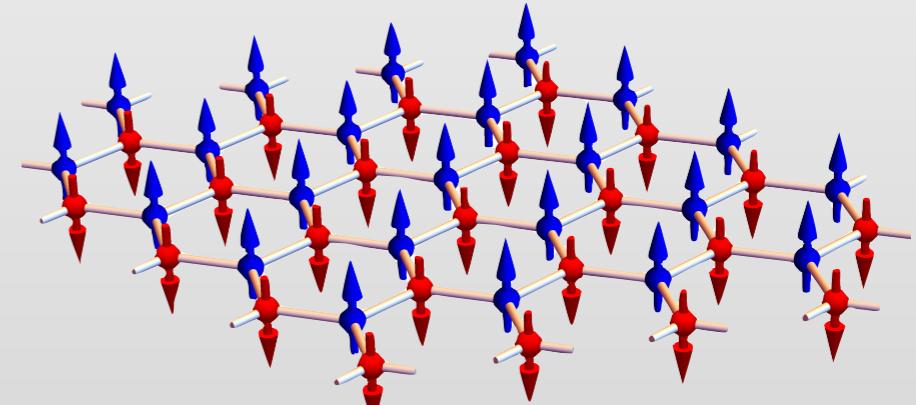
We propose a simple model for a semiconductor-metal transition, based on the existence of both localized (ionic) and band (Bloch) states. It differs from other theories in that we assume the one-electron states to be essentially unchanged by the transition. The electron-hole interaction is responsible for the anomalous temperature dependence of the number of conduction electrons. For interactions larger than a critical value, a first-order semiconductor-metal phase transition takes place.

Long-range spin order on bipartite lattices with infinitesimal repulsion

Kennedy and Lieb 1986

“Fruit fly” of DMFT

Freericks and Zlatić, RMP, 2003

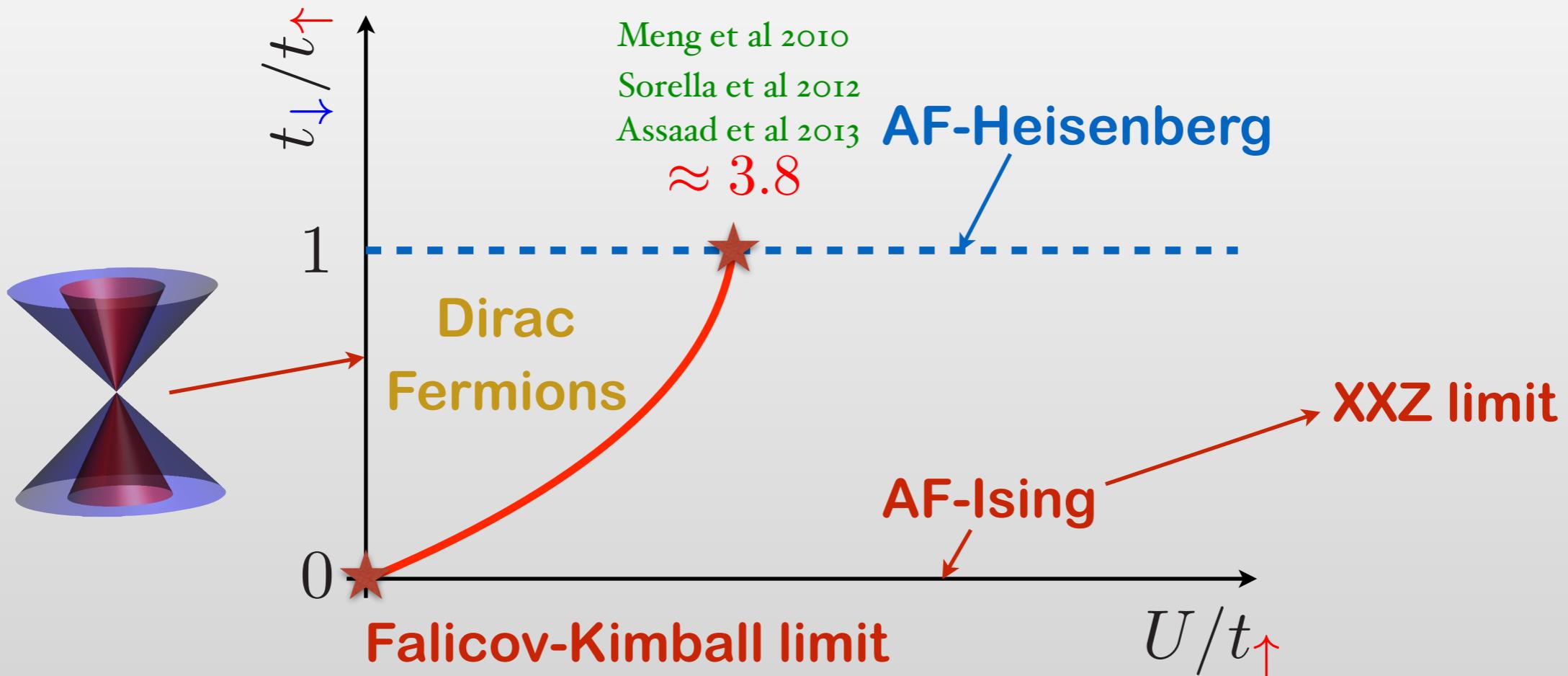


$$J_{xy} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y) + J_z \hat{S}_i^z \hat{S}_j^z$$

$\frac{4t_{\uparrow}t_{\downarrow}}{U} \leq \frac{2(t_{\uparrow}^2 + t_{\downarrow}^2)}{U}$

XXZ model with Ising anisotropy

Phase diagram

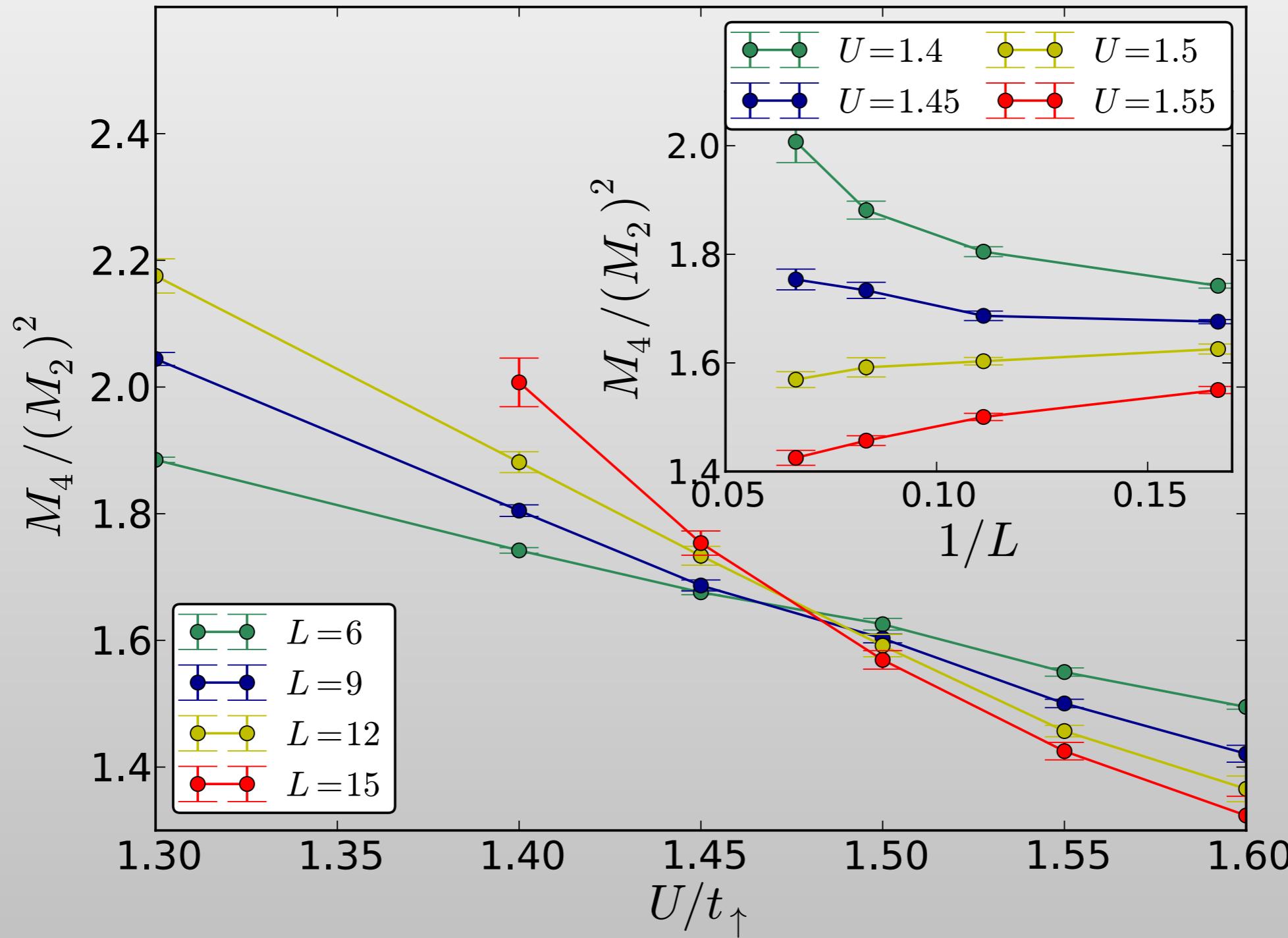


- 📌 How to connect the phase boundary ?
- 📌 What is the universality class ?

Binder ratio

$t_{\downarrow}/t_{\uparrow} = 0.15$

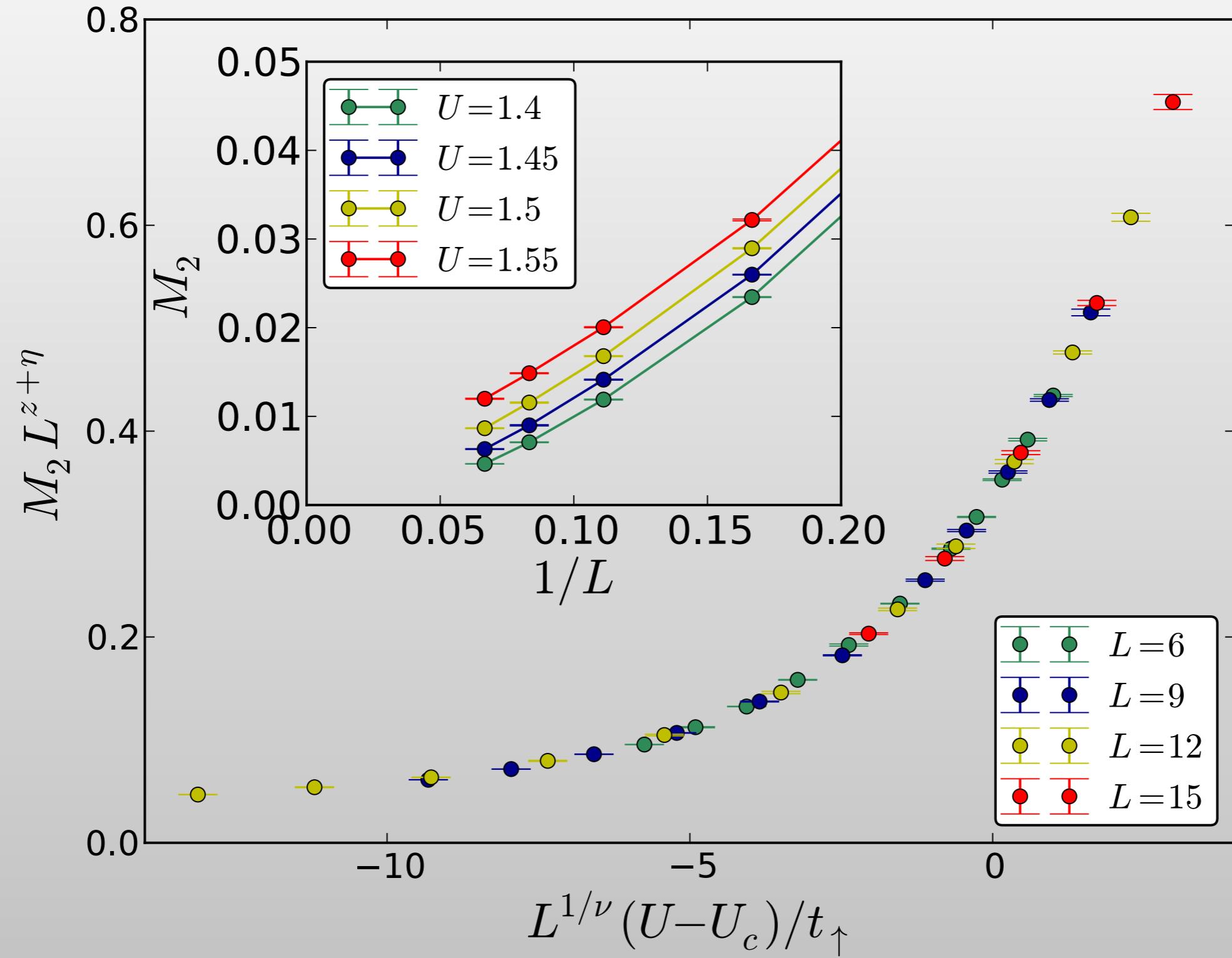
$$M_2 = \left\langle \left(\frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{Q} \cdot \mathbf{r}} \frac{\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}}{2} \right)^2 \right\rangle \quad M_4 = \left\langle \left(\frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{Q} \cdot \mathbf{r}} \frac{\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}}{2} \right)^4 \right\rangle$$



Scaling analysis

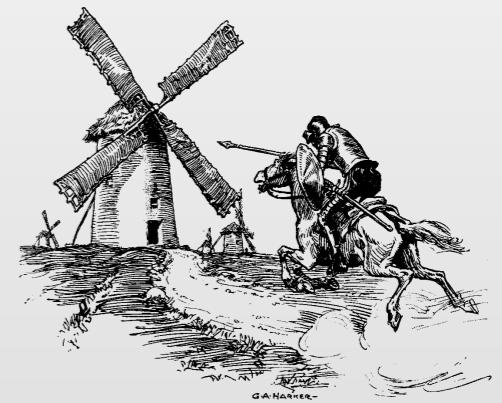
$\nu = 0.84(4)$

$z + \eta = 1.395(7)$



Summary

Exciting time for QMC simulation of lattice fermions



Thanks to my collaborators!

Mauro
Iazzi

Philippe
Corboz

Ye-Hua
Liu

Jakub
Imriška

Ping Nang
Ma

Gergely
Harcos

Matthias
Troyer

